

Propanal

123-38-6 | DTXSID2021658

Model Performance

Model

Data

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.72 | 51.8 | 0.74 | 50.3 | 0.73 | 52.7 |

Model Results

Predicted value: -86.0 °C

Global applicability domain: Inside

Local applicability domain index: 8.17e-01

Confidence level: 7.70e-01

Nearest Neighbors from the Training Set

| | | |
|--|--|---|
| <div>Image not found</div> <div>Propanal</div> <div>Measured: -80.0</div> <div>Predicted: -86.0</div> | <div>Image not found</div> <div>Acetone</div> <div>Measured: -96.6</div> <div>Predicted: -87.6</div> | <div>Image not found</div> <div>(2H6)Acetone</div> <div>Measured: -96.6</div> <div>Predicted: -87.6</div> |
| <div>Image not found</div> <div>Butyraldehyde</div> <div>Measured: -99.0</div> <div>Predicted: -85.8</div> | <div>Image not found</div> <div>Methyl ethyl ketone</div> <div>Measured: -86.6</div> <div>Predicted: -78.1</div> | <div>Image not found</div> <div>2-Methylpropanal</div> <div>Measured: -65.9</div> <div>Predicted: -55.3</div> |